

GPR

GPT-SMILES

GPT-SELFIES

GPT-InChI

TabPFN

accuracy

0.7

0.6

0.5

100

200

300

400

500

F₁ macro

0.6

0.5

0.4

100

200

300

400

500

F₁ micro

0.7

0.6

0.5

100

200

300

400

500

 κ

0.4

0.2

0.0

100

200

300

400

500

number of training points

